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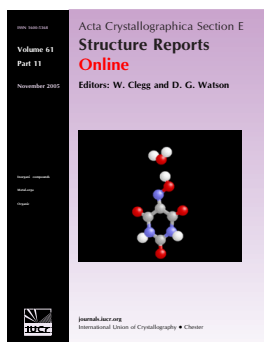
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catena-Poly[[triphenyltin(IV)]- μ -phenylphosphinato- κ^2 O:O']

Tidiane Diop, Libasse Diop, Gabriele Kociok-Köhn, Kieran C. Molloy and Helen Stoeckli-Evans

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catena-Poly[[triphenyltin(IV)]- μ -phenylphosphinato- κ^2 O:O']

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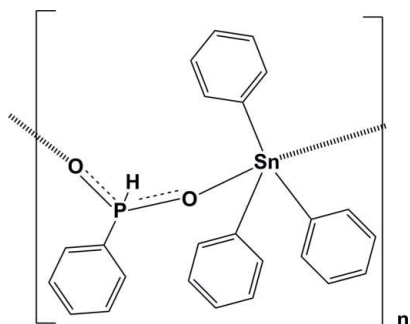
Received 21 September 2011; accepted 20 October 2011

Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}—\text{C}) = 0.009$ Å; R factor = 0.052; wR factor = 0.079; data-to-parameter ratio = 14.9.

In the structure of the title coordination polymer, $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_6\text{H}_5\text{O}_2\text{P})]_n$ or $[\text{PhP}(\text{H})\text{O}_2\text{Sn}^{\text{IV}}(\text{Ph})_3]_n$, the Sn^{IV} atom is five-coordinate, with the SnC_3O_2 framework in a *trans* trigonal-bipyramidal arrangement having the $\text{PhP}(\text{H})\text{O}_2^-$ anions in apical positions. In the crystal, neighbouring polymer chains are linked *via* $\text{C}—\text{H} \cdots \pi$ interactions, forming a two-dimensional network lying parallel to (001).

Related literature

For medical applications of tin(IV) compounds, see: Evans & Karpel (1985); Kapoor *et al.* (2005); Yin & Wang (2004). For literature on new organotin compounds, see: Chandrasekhar *et al.* (2003); Davies & Smith (1982); Zhang *et al.* (2006). For work in this field carried out by the authors, see: Diassé-Sarr *et al.* (1997); Diop *et al.* (2002, 2003); Diallo *et al.* (2009). For related structures, see: Molloy *et al.* (1981); Adair *et al.* (2003).



Experimental

Crystal data

$[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_6\text{H}_5\text{O}_2\text{P})]$
 $M_r = 491.07$
Orthorhombic, $Pbca$
 $a = 14.0108$ (6) Å
 $b = 11.7674$ (7) Å
 $c = 25.7068$ (12) Å

$V = 4238.3$ (4) Å³
 $Z = 8$
Mo $K\alpha$ radiation
 $\mu = 1.30$ mm⁻¹
 $T = 173$ K
 $0.18 \times 0.13 \times 0.10$ mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: multi-scan
(*MULSCAN* in *PLATON*;
Spek, 2009)
 $T_{\min} = 0.973$, $T_{\max} = 1.000$

27270 measured reflections
3829 independent reflections
2467 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.117$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.052$
 $wR(F^2) = 0.079$
 $S = 1.00$
3829 reflections
257 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.47$ e Å⁻³
 $\Delta\rho_{\min} = -0.68$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the C19–C24 ring.

| $D—H \cdots A$ | $D—H$ | $H \cdots A$ | $D \cdots A$ | $D—H \cdots A$ |
|---|-------|--------------|--------------|----------------|
| $\text{C9}—\text{H9} \cdots \text{Cg1}^{\text{i}}$ | 0.95 | 2.79 | 3.656 (9) | 151 |
| $\text{C18}—\text{H18} \cdots \text{Cg1}^{\text{ii}}$ | 0.95 | 2.91 | 3.714 (6) | 143 |

Symmetry codes: (i) $x + \frac{1}{2}, y, -z + \frac{1}{2}$; (ii) $-x - \frac{1}{2}, y + \frac{1}{2}, z$.

Data collection: *X-Area* (Stoe & Cie, 2009); cell refinement: *X-Area*; data reduction: *X-RED32* (Stoe & Cie, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97*, *PLATON* and *publCIF* (Westrip, 2010).

HSE thanks the staff of the X-ray Diffraction Application Laboratory, CSEM, Neuchâtel, for access to the X-ray diffraction equipment.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MW2028).

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supplementary materials

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***catena*-Poly[[triphenyltin(IV)]- μ -phenylphosphinato- $k^2O:O'$]I**

T. Diop, L. Diop, G. Kociok-Köhn, K. C. Molloy and H. Stoeckli-EvansI

Comment

As some compounds belonging to the organotin (IV) family have been found to be the subject of applications in medicine, agriculture, industry (Evans & Karpel, 1985; Kapoor *et al.*, 2005; Yin & Wang, 2004), many groups have been involved in the search for new organotin compounds (Davies & Smith, 1982; Zhang *et al.*, 2006; Chandrasekhar *et al.*, 2003). Our group has published a number of papers in this field (Diassé-Sarr *et al.*, 1997; Diop *et al.*, 2003; Diop *et al.*, 2002; Diallo *et al.*, 2009). In a continuation of this work we initiated the study of the interaction between $Cy_2NH_2PhP(H)O_2$ and $Sn(Ph)_3Cl$, which has led to the synthesis of the title coordination polymer.

The structure of the asymmetric unit of the title compound is illustrated in Fig. 1. The molecular units associate to form an infinite one-dimensional polymer (Fig. 2) in which trimethyltin(IV) groups are axially bridged by $-O-P-O-$ linkages of the phenylphosphinate ligand to yield an almost perfect trigonal bipyramid at the tin(IV) atom; with equatorial location of the phenyl groups and axial disposition of the oxygenated ligand.

The sum of the angles at atom Sn1 by the *ipso*-carbons [124.1 (2), 119.4 (3), 116.4 (3) °] is 359.9°. The corresponding axial O1—Sn—O2 angle is 175.99 (15) °, indicating a slight deviation from linearity. The two axial Sn—O distances, [Sn1—O1 2.241 (4) Å and Sn—O2 2.237 (3) Å], are longer than the Sn—O axial distances [2.116 (2) Å and 2.132 (3) Å] observed in *catena*-(μ_2 -phenylphosphinato- O,O')-chloro-tin(II) [Adair *et al.*, 2003]. The two P—O distances of the bridging O1—P1—O2 moieties are also almost equal [P1—O1 1.514 (4) Å and P1—O2 1.501 (4) Å]. The geometry around the phosphorus atom is a distorted tetrahedron with bond angles ranging from 114.4 (2)° for O1—P1—O2 to 103 (2)° for C1—P1—H1. The P1—H1 distance is 1.33 (5) Å, similar to the same distance, of 1.39 (7) Å, observed in the compound mentioned above.

In the crystal, neighbouring chains are linked *via* C—H $\cdots\pi$ interactions, involving the phenyl ring (C19—C24). This results in the formation of a two-dimensional network structure lying parallel to the *ab*-plane (Table 1 and Fig. 3).

Footnote to Table 1: Cg1 is the centroid of ring (C19—C24).

Experimental

Synthesis: $Cy_2NH_2Ph(H)PO_2$ (*L*) was obtained on neutralizing phenylphosphinic acid with dicyclohexylamine, in 1:2 ratio, in water; a white powder was collected after evaporation at 333 K. When (*L*) was mixed with $Sn(Ph)_3Cl$ (1:1 ratio, *M.p.* +533 K), both in ethanol, a white precipitate formed and the solution was stirred for a further 2 h. The mixture was then filtered and the solid dissolved in 25 ml of slightly hydrated methanol. The solution was then left for the solvent to slowly evaporate giving colourless crystals, suitable for X-ray diffraction analysis, of the title compound. Reaction: $Cy_2NH_2Ph(H)PO_2 + Sn(Ph)_3Cl \rightarrow PhP(H)O_2Sn(Ph)_3 + Cy_2NH_2Cl$. The same compound could be obtained by refluxing trimethyltin chloride with phenylphosphinic acid in water: $Ph(H)PO_2H + Sn(Ph)_3Cl \rightarrow PhP(H)O_2Sn(Ph)_3 + HCl$.

Refinement

The PH H-atom was located in a difference Fourier map and was refined with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{P})$; [P—H = 1.33 (5) Å].
The C-bound H atoms were included in calculated positions and treated as riding atoms: C—H = 0.95 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

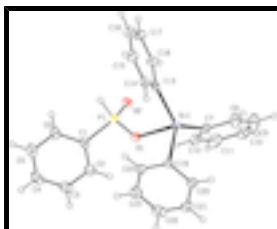


Fig. 1. A view of the asymmetric unit of the title compound, showing the numbering scheme and displacement ellipsoids drawn at the 50% probability level.

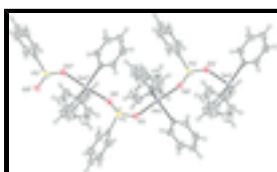


Fig. 2. A view normal to (001) of the polymer chain of the title compound [Symmetry codes: (i) $-x - 1/2, y - 1/2, z$; (ii) $-x - 1/2, y + 1/2, z$; displacement ellipsoids are drawn at the 50% probability level].

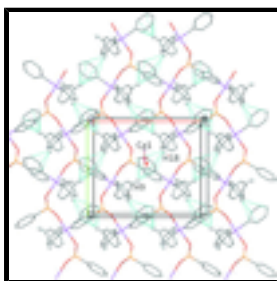


Fig. 3. A view along the c axis of the crystal packing of the title compound showing the weak C—H... π interactions [represented by the H...C dashed cyan lines; Sn violet; P yellow; O red; H grey ball; Cg1 = centroid of ring (C19—C24)].

catena-Poly[[triphenyltin(IV)]- μ -phenylphosphinato- $\kappa^2\text{O}:\text{O}'$]

Crystal data

[Sn(C₆H₅)₃(C₆H₄O₂P)]_n

$M_r = 491.07$

Orthorhombic, $Pbca$

Hall symbol: $-P\ 2ac\ 2abi$

$a = 14.0108$ (6) Å

$b = 11.7674$ (7) Å

$c = 25.7068$ (12) Å

$V = 4238.3$ (4) Å³

$Z = 8$

$F(000) = 1968$.

$D_x = 1.539$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 10452 reflections

$\theta = 1.6\text{--}26.1^\circ$

$\mu = 1.30$ mm⁻¹

$T = 173$ K

Rod, colourless

$0.18 \times 0.13 \times 0.10$ mm

Data collection

| | |
|--|--|
| Stoe IPDS Ili diffractometeri | 3829 independent reflections |
| Radiation source: fine-focus sealed tubei plane graphitei | 2467 reflections with $I > 2\sigma(I)$ i $R_{\text{int}} = 0.117$ i |
| φ and ω scansi | $\theta_{\text{max}} = 25.3^\circ$, $\theta_{\text{min}} = 1.6^\circ$ i |
| Absorption correction: multi-scani (MULscanABS in PLATON; Spek, 2009) | $h = -16 \rightarrow 16$ i |
| $T_{\text{min}} = 0.973$, $T_{\text{max}} = 1.000$ i | $k = -14 \rightarrow 14$ i |
| 27270 measured reflectionsi | $l = -28 \rightarrow 30$ i |

Refinement

| | |
|---|---|
| Refinement on F^2 i | Secondary atom site location: difference Fourier mapsi |
| Least-squares matrix: fulli | Hydrogen site location: inferred from neighbouring sitesi |
| $R[F^2 > 2\sigma(F^2)] = 0.052$ i | H atoms treated by a mixture of independent and constrained refinementi |
| $wR(F^2) = 0.079$ | $w = 1/[\sigma^2(F_o^2) + (0.0275i)^2]$ i where $i = (F_o^2 + 2F_c^2)/3$ i |
| $S = 1.00$ i | $(\Delta/\sigma)_{\text{max}} = 0.001$ i |
| 3829 reflectionsi | $\Delta\rho_{\text{max}} = 0.47 \text{ e } \text{\AA}^{-3}$ i |
| 257 parameterisi | $\Delta\rho_{\text{min}} = -0.68 \text{ e } \text{\AA}^{-3}$ i |
| 0 restraintsi | Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$ i |
| Primary atom site location: structure-invariant directi methodsi | Extinction coefficient: 0.00036 (5)i |

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion anglesi

Refinement. The PH H-atom was located in a difference Fourier map and was refined with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{P})$. The C-bound H-i atoms were included in calculated positions and treated as riding atoms: C—H = 0.95 Å for CH(aromatic), with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.i

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eqi}}$ |
|------|----------------|----------------|---------------|-----------------------------------|
| Sn1i | −0.29327 (3)i | −0.35558 (3)i | 0.36284 (1)i | 0.0260 (1)i |
| P1i | −0.36921 (12)i | −0.08232 (12)i | 0.38935 (6)i | 0.0286 (5)i |
| O1i | −0.3855 (3)i | −0.2003 (3)i | 0.36764 (17)i | 0.0295 (11)i |
| O2i | −0.2923 (3)i | −0.0161 (2)i | 0.36231 (17)i | 0.0350 (11)i |
| C1i | −0.4806 (4)i | −0.0060 (4)i | 0.3878 (3)i | 0.029 (2)i |
| C2i | −0.5372 (5)i | −0.0034 (5)i | 0.3438 (3)i | 0.047 (3)i |
| C3i | −0.6217 (5)i | 0.0586 (6)i | 0.3440 (3)i | 0.053 (3)i |

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| | | | | |
|------|--------------|--------------|-------------|--------------|
| C4i | −0.6498 (5)i | 0.1153 (5)i | 0.3884 (3)i | 0.052 (3)i |
| C5i | −0.5930 (5)i | 0.1151 (5)i | 0.4317 (3)i | 0.050 (3)i |
| C6i | −0.5077 (5)i | 0.0548 (5)i | 0.4313 (3)i | 0.040 (2)i |
| C7i | −0.2349 (4)i | −0.3088 (5)i | 0.2893 (2)i | 0.0317 (19) |
| C8i | −0.1608 (5)i | −0.3689 (6)i | 0.2669 (3)i | 0.050 (3)i |
| C9 | −0.1227 (6)i | −0.3364 (7)i | 0.2197 (3)i | 0.065 (3)i |
| C10i | −0.1576 (6)i | −0.2451 (6)i | 0.1937 (3)i | 0.054 (3)i |
| C11i | −0.2315 (6)i | −0.1838 (6)i | 0.2150 (3)i | 0.059 (3)i |
| C12i | −0.2705 (5)i | −0.2148 (5)i | 0.2623 (2)i | 0.041 (2)i |
| C13i | −0.2300 (4)i | −0.3139 (4)i | 0.4356 (2)i | 0.0260 (18)i |
| C14i | −0.2518 (5)i | −0.3764 (4)i | 0.4803 (2)i | 0.0323 (17)i |
| C15i | −0.2086 (5)i | −0.3528 (5)i | 0.5273 (2)i | 0.0400 (17)i |
| C16i | −0.1414 (5)i | −0.2654 (5)i | 0.5310 (3)i | 0.042 (3)i |
| C17i | −0.1206 (5)i | −0.2024 (5)i | 0.4872 (2)i | 0.039 (2)i |
| C18i | −0.1629 (4)i | −0.2252 (5)i | 0.4404 (2)i | 0.0327 (19) |
| C19 | −0.4177 (4)i | −0.4597 (4)i | 0.3655 (3)i | 0.0273 (16)i |
| C20i | −0.4303 (5)i | −0.5480 (5)i | 0.3302 (3)i | 0.038 (2)i |
| C21i | −0.5101 (5)i | −0.6171 (5)i | 0.3344 (3)i | 0.047 (3)i |
| C22i | −0.5766 (5)i | −0.5986 (5)i | 0.3719 (3)i | 0.050 (3)i |
| C23i | −0.5660 (5)i | −0.5107 (6)i | 0.4068 (3)i | 0.048 (3)i |
| C24i | −0.4866 (4)i | −0.4413 (5)i | 0.4031 (2)i | 0.034 (2)i |
| H1i | −0.351 (4)i | −0.089 (4)i | 0.440 (2)i | 0.0340*i |
| H2i | −0.51850i | −0.04380i | 0.31350i | 0.0570*i |
| H3i | −0.66010i | 0.06180i | 0.31360i | 0.0640*i |
| H4i | −0.70900i | 0.15470i | 0.38890i | 0.0620*i |
| H5i | −0.61170i | 0.15600i | 0.46190i | 0.0590*i |
| H6i | −0.46790i | 0.05530i | 0.46120i | 0.0480*i |
| H8i | −0.13570i | −0.43360i | 0.28430i | 0.0600*i |
| H9 | −0.07140i | −0.37860i | 0.20510i | 0.0770*i |
| H10i | −0.13120i | −0.22350i | 0.16120i | 0.0650*i |
| H11i | −0.25600i | −0.11970i | 0.19700i | 0.0710*i |
| H12i | −0.32180i | −0.17200i | 0.27650i | 0.0500*i |
| H14i | −0.29720i | −0.43620i | 0.47820i | 0.0390*i |
| H15i | −0.22460i | −0.39600i | 0.55730i | 0.0480*i |
| H16i | −0.11060i | −0.24970i | 0.56310i | 0.0510*i |
| H17i | −0.07590i | −0.14200i | 0.48960i | 0.0460*i |
| H18i | −0.14700i | −0.18070i | 0.41070i | 0.0390*i |
| H20i | −0.38480i | −0.56080i | 0.30350i | 0.0450*i |
| H21i | −0.51820i | −0.67840i | 0.31080i | 0.0570*i |
| H22i | −0.63100i | −0.64670i | 0.37400i | 0.0600*i |
| H23i | −0.61240i | −0.49800i | 0.43310i | 0.0570*i |
| H24i | −0.47930i | −0.37990i | 0.42670i | 0.0410*i |

Atomic displacement parameters (\AA^2)

| | U^{11i} | U^{22i} | U^{33i} | U^{12i} | U^{13i} | U^{23i} |
|------|-------------|-------------|-------------|--------------|--------------|--------------|
| Sn1i | 0.0255 (2)i | 0.0192 (2)i | 0.0334 (2)i | −0.0004 (2)i | 0.0006 (2)i | 0.0008 (2)i |
| P1i | 0.0288 (9) | 0.0191 (7)i | 0.0380 (9) | −0.0004 (7)i | −0.0023 (8)i | −0.0018 (7)i |

| | | | | | | |
|------|------------|--------------|------------|---------------|-------------|---------------|
| O1i | 0.031 (2)i | 0.0156 (16)i | 0.042 (2)i | −0.0002 (15)i | −0.002 (2)i | −0.0021 (18)i |
| O2i | 0.029 (2)i | 0.0209 (16)i | 0.055 (2)i | −0.0052 (18)i | 0.002 (3)i | −0.0016 (19)i |
| C1i | 0.027 (4)i | 0.014 (3)i | 0.047 (4)i | 0.002 (3)i | 0.002 (3)i | 0.003 (3)i |
| C2i | 0.041 (5)i | 0.037 (3)i | 0.064 (5)i | 0.006 (3)i | −0.010 (4)i | −0.012 (3)i |
| C3i | 0.042 (5)i | 0.041 (4)i | 0.076 (5)i | 0.008 (3)i | −0.018 (4)i | 0.003 (4)i |
| C4i | 0.033 (4)i | 0.026 (4)i | 0.096 (6)i | 0.004 (3)i | 0.007 (4)i | 0.003 (3)i |
| C5i | 0.044 (5)i | 0.041 (4)i | 0.064 (5)i | 0.006 (3)i | 0.015 (4)i | −0.001 (3)i |
| C6i | 0.041 (4)i | 0.031 (3)i | 0.048 (4)i | 0.006 (3)i | 0.006 (3)i | 0.002 (3)i |
| C7i | 0.036 (4)i | 0.025 (3)i | 0.034 (3)i | −0.003 (3)i | 0.001 (3)i | −0.001 (3)i |
| C8i | 0.061 (5)i | 0.041 (4)i | 0.048 (4)i | 0.005 (4)i | 0.013 (4)i | 0.003 (3)i |
| C9 | 0.076 (6)i | 0.065 (5)i | 0.053 (5)i | 0.001 (5)i | 0.030 (4)i | 0.001 (4)i |
| C10i | 0.070 (6)i | 0.063 (5)i | 0.030 (4)i | −0.022 (4)i | 0.010 (4)i | 0.000 (4)i |
| C11i | 0.086 (7)i | 0.052 (4)i | 0.040 (4)i | −0.009 (4)i | −0.005 (4)i | 0.007 (3)i |
| C12i | 0.053 (5)i | 0.036 (3)i | 0.035 (4)i | 0.003 (3)i | −0.006 (3)i | −0.006 (3)i |
| C13i | 0.027 (4)i | 0.017 (2)i | 0.034 (3)i | 0.005 (2)i | 0.004 (3)i | −0.001 (2)i |
| C14i | 0.035 (3)i | 0.019 (3)i | 0.043 (3)i | −0.001 (2)i | 0.006 (3)i | 0.003 (2)i |
| C15i | 0.043 (3)i | 0.045 (3)i | 0.032 (3)i | −0.001 (4)i | 0.002 (3)i | 0.007 (3)i |
| C16i | 0.045 (5)i | 0.045 (4)i | 0.037 (4)i | −0.004 (3)i | −0.006 (3)i | 0.000 (3)i |
| C17i | 0.044 (4)i | 0.031 (3)i | 0.041 (4)i | −0.010 (3)i | −0.008 (3)i | 0.004 (3)i |
| C18i | 0.036 (4)i | 0.031 (3)i | 0.031 (3)i | −0.003 (3)i | −0.004 (3)i | 0.005 (3)i |
| C19 | 0.030 (3)i | 0.015 (2)i | 0.037 (3)i | 0.001 (2)i | −0.010 (4)i | 0.001 (3)i |
| C20i | 0.035 (4)i | 0.030 (3)i | 0.048 (4)i | 0.000 (3)i | −0.003 (3)i | −0.008 (3)i |
| C21i | 0.051 (5)i | 0.026 (4)i | 0.064 (5)i | −0.007 (3)i | −0.012 (4)i | −0.012 (3)i |
| C22i | 0.041 (4)i | 0.034 (3)i | 0.075 (6)i | −0.014 (3)i | −0.005 (4)i | 0.009 (4)i |
| C23i | 0.040 (5)i | 0.045 (4)i | 0.059 (5)i | −0.013 (3)i | 0.005 (4)i | 0.002 (4)i |
| C24i | 0.031 (4)i | 0.030 (3)i | 0.042 (4)i | −0.006 (3)i | 0.002 (3)i | −0.006 (3)i |

Geometric parameters (Å, °)

| | | | |
|----------|-------------|----------|-------------|
| Sn1—O1i | 2.241 (4)i | C19—C24i | 1.383 (9)i |
| Sn1—C7i | 2.132 (5)i | C19—C20i | 1.391 (9)i |
| Sn1—C13i | 2.127 (5)i | C20—C21i | 1.387 (9)i |
| Sn1—C19 | 2.132 (5)i | C21—C22i | 1.358 (10)i |
| Sn1—O2i | 2.237 (3)i | C22—C23i | 1.377 (10)i |
| P1—O1i | 1.514 (4)i | C23—C24i | 1.383 (9)i |
| P1—O2i | 1.501 (4)i | C2—H2i | 0.9500i |
| P1—C1i | 1.801 (6)i | C3—H3i | 0.9500i |
| P1—H1i | 1.33 (5)i | C4—H4i | 0.9500i |
| C1—C2i | 1.382 (10)i | C5—H5i | 0.9500i |
| C1—C6i | 1.381 (10)i | C6—H6i | 0.9500i |
| C2—C3i | 1.391 (10)i | C8—H8i | 0.9500i |
| C3—C4i | 1.380 (10)i | C9—H9 | 0.9500i |
| C4—C5i | 1.368 (11)i | C10—H10i | 0.9500i |
| C5—C6i | 1.390 (10)i | C11—H11i | 0.9500i |
| C7—C12i | 1.398 (8)i | C12—H12i | 0.9500i |
| C7—C8i | 1.382 (9)i | C14—H14i | 0.9500i |
| C8—C9 | 1.380 (11)i | C15—H15i | 0.9500i |
| C9—C10i | 1.357 (11)i | C16—H16i | 0.9500i |
| C10—C11i | 1.376 (11)i | C17—H17i | 0.9500i |

supplementary materials

| | | | |
|--------------|--------------|--------------|------------|
| C11—C12i | 1.382 (10)i | C18—H18i | 0.9500i |
| C13—C14i | 1.398 (7)i | C20—H20i | 0.9500i |
| C13—C18i | 1.410 (8)i | C21—H21i | 0.9500i |
| C14—C15i | 1.380 (8)i | C22—H22i | 0.9500i |
| C15—C16i | 1.398 (9)i | C23—H23i | 0.9500i |
| C16—C17i | 1.379 (9)i | C24—H24i | 0.9500i |
| C17—C18i | 1.368 (8)i | | |
| O1—Sn1—C7i | 93.41 (19) | C19—C20—C21i | 119.3 (7)i |
| O1—Sn1—C13i | 90.22 (17)i | C20—C21—C22i | 121.0 (6)i |
| O1—Sn1—C19 | 89.73 (17)i | C21—C22—C23i | 120.6 (6)i |
| O1—Sn1—O2i | 175.99 (15)i | C22—C23—C24i | 119.0 (6)i |
| C7—Sn1—C13i | 124.1 (2)i | C19—C24—C23i | 121.1 (6)i |
| C7—Sn1—C19 | 119.4 (3)i | C1—C2—H2i | 120.00i |
| O2i—Sn1—C7i | 90.41 (19) | C3—C2—H2i | 120.00i |
| C13—Sn1—C19 | 116.4 (3)i | C2—C3—H3i | 120.00i |
| O2i—Sn1—C13i | 88.66 (17)i | C4—C3—H3i | 120.00i |
| O2i—Sn1—C19 | 87.32 (17)i | C3—C4—H4i | 120.00i |
| O1—P1—O2i | 114.4 (2)i | C5—C4—H4i | 120.00i |
| O1—P1—C1i | 108.6 (3)i | C4—C5—H5i | 120.00i |
| O2—P1—C1i | 110.7 (2)i | C6—C5—H5i | 120.00i |
| O1—P1—H1i | 110 (2)i | C1—C6—H6i | 120.00i |
| O2—P1—H1i | 110 (2)i | C5—C6—H6i | 120.00i |
| C1—P1—H1i | 103 (2)i | C7—C8—H8i | 119.00i |
| Sn1—O1—P1i | 132.9 (3)i | C9—C8—H8i | 120.00i |
| Sn1i—O2—P1i | 145.1 (2)i | C8—C9—H9 | 120.00i |
| P1—C1—C2i | 121.8 (5)i | C10—C9—H9 | 119.00i |
| C2—C1—C6i | 119.6 (6)i | C9—C10—H10i | 120.00i |
| P1—C1—C6i | 118.6 (5)i | C11—C10—H10i | 120.00i |
| C1—C2—C3i | 119.8 (7)i | C10—C11—H11i | 120.00i |
| C2—C3—C4i | 120.0 (7)i | C12—C11—H11i | 120.00i |
| C3—C4—C5i | 120.4 (6)i | C7—C12—H12i | 120.00i |
| C4—C5—C6i | 119.7 (7)i | C11—C12—H12i | 120.00i |
| C1—C6—C5i | 120.5 (7)i | C13—C14—H14i | 119.00i |
| Sn1—C7—C8i | 121.7 (5)i | C15—C14—H14i | 120.00i |
| Sn1—C7—C12i | 120.5 (4)i | C14—C15—H15i | 120.00i |
| C8—C7—C12i | 117.8 (5)i | C16—C15—H15i | 120.00i |
| C7—C8—C9 | 121.0 (7)i | C15—C16—H16i | 121.00i |
| C8—C9—C10i | 120.9 (7)i | C17—C16—H16i | 121.00i |
| C9—C10—C11i | 119.4 (7)i | C16—C17—H17i | 119.00i |
| C10—C11—C12i | 120.6 (7)i | C18—C17—H17i | 119.00i |
| C7—C12—C11i | 120.3 (6)i | C13—C18—H18i | 120.00i |
| Sn1—C13—C14i | 120.7 (4)i | C17—C18—H18i | 120.00i |
| C14—C13—C18i | 117.6 (5)i | C19—C20—H20i | 120.00i |
| Sn1—C13—C18i | 121.7 (4)i | C21—C20—H20i | 120.00i |
| C13—C14—C15i | 121.2 (5)i | C20—C21—H21i | 119.00i |
| C14—C15—C16i | 120.2 (6)i | C22—C21—H21i | 120.00i |
| C15—C16—C17i | 118.8 (6)i | C21—C22—H22i | 120.00i |
| C16—C17—C18i | 121.4 (6)i | C23—C22—H22i | 120.00i |

| | | | |
|------------------|-------------|------------------|-------------|
| C13—C18—C17i | 120.7 (5)i | C22—C23—H23i | 121.00i |
| Sn1—C19—C20i | 120.8 (5)i | C24—C23—H23i | 120.00i |
| Sn1—C19—C24i | 120.2 (4)i | C19—C24—H24i | 119.00i |
| C20—C19—C24i | 119.0 (5)i | C23—C24—H24i | 119.00i |
| C7—Sn1—O1—P1i | −89.4 (4)i | O1—P1—C1—C6i | 134.2 (5)i |
| C13—Sn1—O1—P1i | 34.8 (4)i | O2—P1—C1—C2i | 78.1 (5)i |
| C19—Sn1—O1—P1i | 151.2 (4)i | O2—P1—C1—C6i | −99.4 (5)i |
| O1—Sn1—C7—C8i | 172.5 (5)i | P1—C1—C2—C3i | −178.7 (5)i |
| O1—Sn1—C7—C12i | −7.0 (5)i | C6—C1—C2—C3i | −1.2 (9)i |
| C13—Sn1—C7—C8i | 79.9 (6)i | P1—C1—C6—C5i | 179.9 (5)i |
| C13—Sn1—C7—C12i | −99.6 (5)i | C2—C1—C6—C5i | 2.3 (9)i |
| C19—Sn1—C7—C8i | −95.9 (5)i | C1—C2—C3—C4i | −1.4 (10)i |
| C19—Sn1—C7—C12i | 84.6 (5)i | C2—C3—C4—C5i | 2.8 (10)i |
| O2i—Sn1—C7—C8i | −8.7 (5)i | C3—C4—C5—C6i | −1.7 (10)i |
| O2i—Sn1—C7—C12i | 171.8 (5)i | C4—C5—C6—C1i | −0.9 (10)i |
| O1—Sn1—C13—C14i | 107.3 (5)i | Sn1—C7—C8—C9 | −178.9 (6)i |
| O1—Sn1—C13—C18i | −74.6 (4)i | C12—C7—C8—C9 | 0.6 (10)i |
| C7—Sn1—C13—C14i | −158.4 (4)i | Sn1—C7—C12—C11i | 179.1 (5)i |
| C7—Sn1—C13—C18i | 19.7 (5)i | C8—C7—C12—C11i | −0.5 (9)i |
| C19—Sn1—C13—C14i | 17.5 (5)i | C7—C8—C9—C10i | −0.7 (12)i |
| C19—Sn1—C13—C18i | −164.4 (4)i | C8—C9—C10—C11i | 0.5 (12)i |
| O2i—Sn1—C13—C14i | −68.9 (5)i | C9—C10—C11—C12i | −0.3 (12)i |
| O2i—Sn1—C13—C18i | 109.3 (4)i | C10—C11—C12—C7i | 0.3 (11)i |
| O1—Sn1—C19—C20i | 132.0 (5)i | Sn1—C13—C14—C15i | 177.6 (5)i |
| O1—Sn1—C19—C24i | −49.1 (5)i | C18—C13—C14—C15i | −0.6 (9)i |
| C7—Sn1—C19—C20i | 38.2 (6)i | Sn1—C13—C18—C17i | −177.7 (5)i |
| C7—Sn1—C19—C24i | −142.8 (5)i | C14—C13—C18—C17i | 0.5 (8)i |
| C13—Sn1—C19—C20i | −137.9 (5)i | C13—C14—C15—C16i | −0.2 (10)i |
| C13—Sn1—C19—C24i | 41.0 (5)i | C14—C15—C16—C17i | 1.1 (10)i |
| O2i—Sn1—C19—C20i | −50.8 (5)i | C15—C16—C17—C18i | −1.3 (10)i |
| O2i—Sn1—C19—C24i | 128.2 (5)i | C16—C17—C18—C13i | 0.5 (9)i |
| C7—Sn1—O2i—P1i | 117.5 (5)i | Sn1—C19—C20—C21i | 177.3 (5)i |
| C13—Sn1—O2i—P1i | −6.6 (4)i | C24—C19—C20—C21i | −1.7 (10)i |
| C19—Sn1—O2i—P1i | −123.2 (5)i | Sn1—C19—C24—C23i | −177.4 (5)i |
| O2—P1—O1—Sn1i | 63.4 (4)i | C20—C19—C24—C23i | 1.6 (9)i |
| C1—P1—O1—Sn1i | −172.4 (4)i | C19—C20—C21—C22i | 1.0 (10)i |
| O1—P1—O2—Sn1i | −174.3 (4)i | C20—C21—C22—C23i | −0.2 (11)i |
| C1—P1—O2—Sn1i | 62.6 (5)i | C21—C22—C23—C24i | 0.1 (11)i |
| O1—P1—C1—C2i | −48.3 (6)i | C22—C23—C24—C19 | −0.8 (10)i |

Symmetry codes: (i) $-x-1/2, y-1/2, z$; (i) $-x-1/2, y+1/2, z$.

Hydrogen-bond geometry (\AA , $^\circ$)

| | | | | |
|-----------------------|--------|-------------|-------------|---------------|
| $D-H\cdots A$ | $D-Hi$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
| C9—H9 \cdots Cg1i | 0.95i | 2.79 | 3.656 (9) | 151i |
| C18—H18 \cdots Cg1i | 0.95i | 2.91i | 3.714 (6)i | 143i |

Symmetry codes: (i) $x+1/2, y, -z+1/2$; (ii) $-x-1/2, y+1/2, z$

Fig. 1

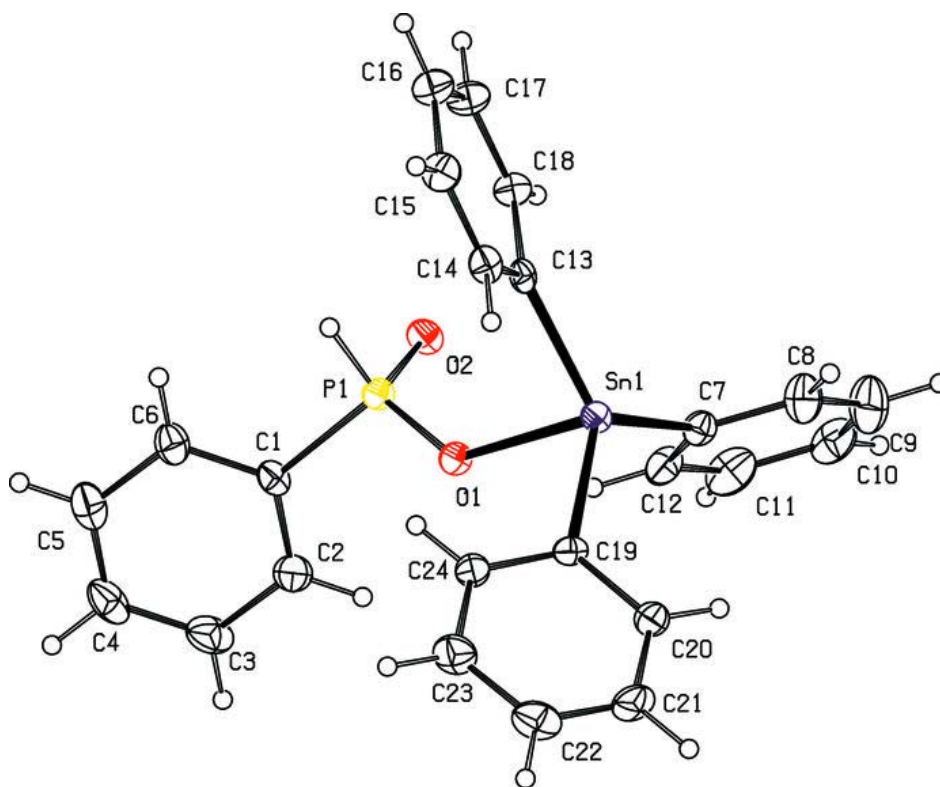


Fig. 2m

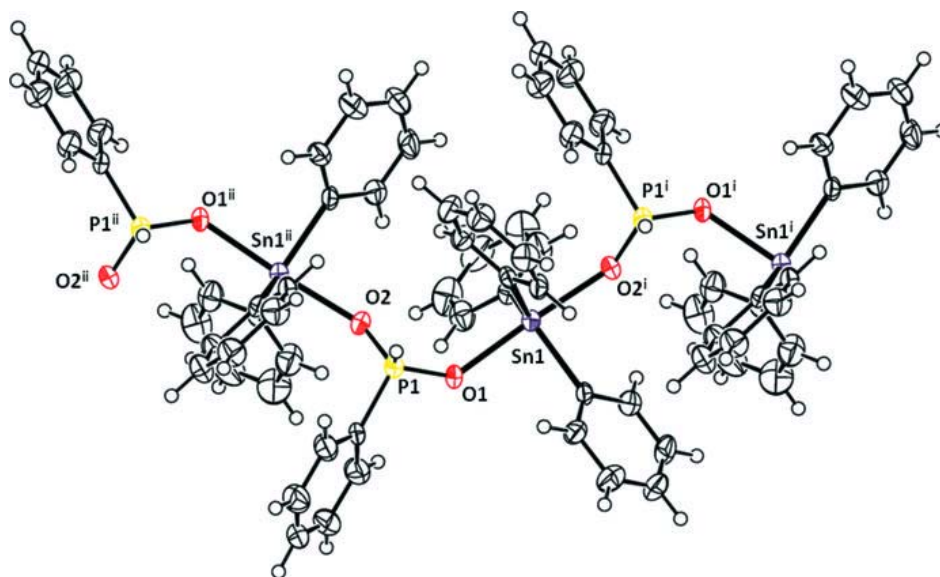


Fig. 3m

